

Heptafluorobutyric acid  
375-22-4 | DTXSID4059916

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 120 °C

Global applicability domain: Inside

Local applicability domain index: 3.55e-01

Confidence level: 6.29e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptafluorobutyric acid</div> <div>Measured: 121</div> <div>Predicted: 120</div>	<div>Image not found</div> <div>Pentafluoropropionic acid</div> <div>Measured: 96.5</div> <div>Predicted: 100</div>	<div>Image not found</div> <div>Flupropanate</div> <div>Measured: 134</div> <div>Predicted: 126</div>
<div>Image not found</div> <div>Acetic acid, trifluoro-</div> <div>Measured: 73.0</div> <div>Predicted: 85.2</div>	<div>Image not found</div> <div>Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7- dodecafluoro-</div> <div>Measured: 192</div> <div>Predicted: 186</div>	